computationally costly compared to simple central difference methods. In this paper we develop a filtering method which uses simple central differencing of arbitrarily high order accuracy, except when a novel local test indicates the development of spurious oscillations. At these points, generally few in number, we use the full ENO apparatus, maintaining (in fact, improving) the high order of accuracy, but removing spurious oscillations. Numerical results indicate the success of the method. We obtain high order of accuracy in regions of smooth flow without spurious oscillations for a wide range of problems and a significant speedup of, generally, a factor of almost three over the full ENO method.

THE ELECTRIC POTENTIAL OF A MACROMOLECULE IN A SOLVENT: A FUNDAMENTAL APPROACH. Andre H. Juffer and Herman J. C. Berendsen, *Laboratory of Physical Chemistry, University of Groningen, Nijenborgh 16, 9747 AG Groningen, THE NETHERLANDS*; Eugen F. F. Botta, Bert A. M. van Keulen, and Auke van der Ploeg, *Department of Mathematics, University of Groningen, P.O. Box 800, 9700 AV Groningen, THE NETHERLANDS.*

A general numerical method is presented to compute the electric potential for a macromolecule of arbitrary shape in a solvent with nonzero ionic strength. The model is based on a continuum description of the dielectric and screening properties of the system, which consists of a bounded internal region with discrete charges and an infinite external region. The potential obeys the Poisson equation in the internal region and the linearized Poisson–Boltzmann equation in the external region, coupled through appropriate boundary conditions. It is shown how this three-dimensional problem can be presented as a pair of coupled integral equations for the potential and the normal component of the electric field at the dielectric interface. These equations can be solved by a straightforward application of boundary element techniques. The solution involves the decomposition of a matrix that depends only on the geometry of the surface and not on the positions of the charges. With this approach the number of unknowns is reduced by an order of magnitude with respect to the usual finite difference methods. Special attention is given to the numerical inaccuracies resulting from charges which are located close to the interface; an adapted formulation is given for that case. The method is tested both for a spherical geometry, for which an exact solution is available, and for a realistic problem, for which a finite difference solution and experimental verification is available. The latter concerns the shift in acid strength (pH-values) of histidines in the copper-containing protein azurin on oxidation of the copper, for various values of the ionic strength. A general method is given to triangulate a macromolecular surface. The possibility is discussed to use the method presented here for a correct treatment of long-range electrostatic interactions in simulations of solvated macromolecules, which form an essential part of correct potentials of mean force.

VORTICITY ERRORS IN MULTIDIMENSIONAL LAGRANGIAN CODES. John K. Dukowicz, *Theoretical Division, Los Alamos National Laboratory, Group T-3, MS B216, Los Alamos, New Mexico 87545, U.S.A.*; Bertrand J. A. Meltz, *Département de Mathématiques Appliqués, Centre d'Etudes de Limeil-Valenton, B.P. 27, 94195 Villeneuve Saint-Georges Cedex, FRANCE.*

We investigate the apparent paradox, as exemplified by the well-known Saltzman test problem of multidimensional lagrangian codes experiencing mesh tangling when computing one-dimensional irrotational flows. We demonstrate that the cause is the generation of spurious vorticity, or vorticity error, by a nonuniform mesh. Based on this, we investigate two methods of constructing improved lagrangian vertex velocities by removing, or filtering out, this spurious vorticity, rather than by the more common practice of introducing artificial viscosity. The first method reconstructs the velocity from the known flow divergence and from the true vorticity computed by means of a transport equation. The second method, which is much simpler and more efficient, subtracts a divergence-free correction from the velocity, such that the resulting velocity possesses the correct vorticity. We then successfully apply this method to solve a two-dimensional shock refraction problem, a problem which exhibits nonzero intrinsic vorticity.